

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.53×10^{-11} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.41×10^{-1}

Confidence level: 7.67×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Cycloate

Measured: 3.54×10^{-11}

Predicted: 2.98×10^{-11}

Image not found

Isoproturon

Measured: 1.20×10^{-11}

Predicted: 3.23×10^{-11}

Image not found

EPTC

Measured: 3.18×10^{-11}

Predicted: 2.83×10^{-11}

Image not found

Bornyl acetate

Measured: 1.39×10^{-11}

Predicted: 1.36×10^{-11}

Image not found

Triethyl phosphate

Measured: 5.53×10^{-11}

Predicted: 4.26×10^{-11}